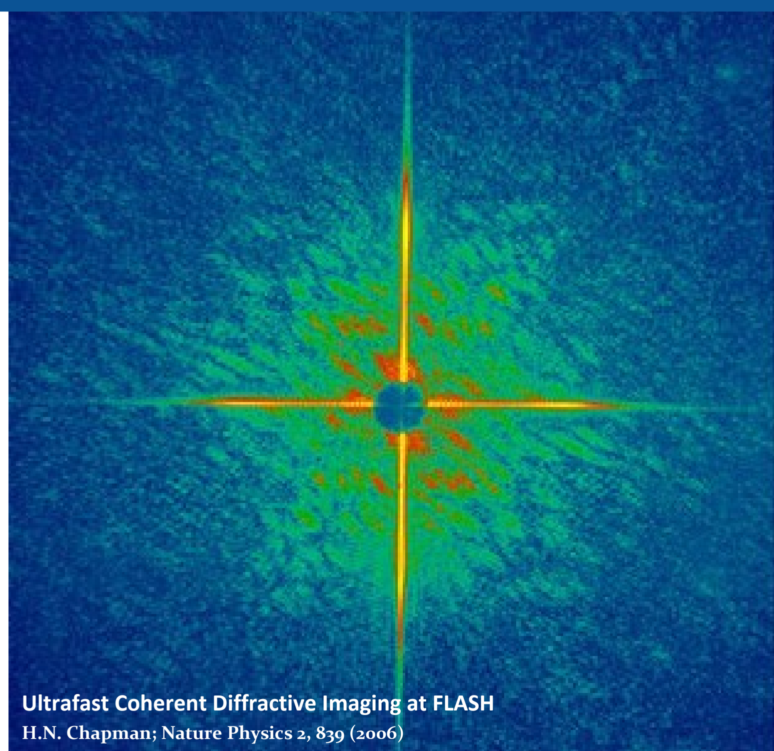
CUI THE HAMBURG CENTRE FOR ULTRAFAST IMAGING

2014

Winter School



Ultrafast Coherent Diffractive Imaging at FLASH
H.N. Chapman; Nature Physics 2, 839 (2006)

Weissenhäuser Strand

(Germany)

01.12 – 05.12.2014

Universität Hamburg DER FORSCHUNG | DER LEHRE | DER BILDUNG

DESY

European XFEL

EMBL

DFG

The Hamburg Centre for Ultrafast Imaging

How do the elementary building blocks of nature move? Can atoms, molecules and electrons in matter be controlled and driven with precision on all length and time scales?
These questions represent some of the biggest and most exciting challenges of modern science – and the central objective of The Hamburg Centre for Ultrafast Imaging (CUI): The analysis of fundamental chemical and physical processes in Photon and Nano Science
The scientists of CUI hope to gain profound insight into fundamental phenomena such as the mechanisms of high temperature superconductivity, the appearance of different states of magnetism or the development of ordered molecular as well as biological and mesoscopic structures. The expected insights will extend and broaden our understanding of physics, chemistry and biology and will result in new applications in medicine and novel materials for key technology areas.

Research Area A (Imaging and Control of Quantum Systems):

For a full understanding of structural dynamics, one needs information on the electronic as well as the nuclear degrees of freedom. This research focus uses advanced optical imaging techniques to identify key enabling features for controlling quantum state evolution. We envisage the possibility to control chemistry along the ground state electronic surface to open up all classes of molecular systems to atomic level inspection. The system size is scaled up from small molecules to collective effects in solid state or periodic media and includes the systematic study of isolated molecules with small potential barriers separating different structures but also takes into account a variable coupling of a system to the environment. With a detailed understanding of electronic coupling to the bath we shall be able to control coherence and degree of dissipation to the point of controlling material properties. For the case of highly correlated electron-lattice systems, this knowledge will lead to new means to control coherence and macroscopic properties with the prospect to eventually create transient superconducting states at high temperatures. The design of novel materials with unique properties are greatly aided by our capabilities to build fully controllable quantum simulators based on periodic structures formed in ultracold quantum gases. In these analog quantum processors ultracold matter is tailored to mimic magnetism and superconductivity under idealized conditions. Apart from the long range correlation effects governing material properties, there is a deep fundamental issue related to the role of quantum information transport in such highly quantized systems. To this end, we are studying the coherence properties of matter waves escaping from a macroscopic quantum object like a Bose-Einstein condensate.

Research Area B (Atomically Resolved Structural Dynamics):

A particular dream experiment is to directly watch atomic motions during a chemical event, such as a bond breaking. With the advent of ultrabright electron and x-ray sources, this has become possible. Techniques such as coherent imaging will allow us to directly watch atomic motions in complex systems, such as in a biological reaction or collective dynamics in a condensed matter system. In this research area we bring together multidisciplinary expertise in laser science, structural biology, chemistry, molecular physics, and imaging science and focus on the basic underlying concepts of systems from small molecules to amino acids and to protein complexes.

Research Area C (Dynamics of Order Formation on the Nanoscale):

Research Area C extends the length scale of interest from the molecular level to the nanoscale where collective effects play a defining role in material properties. The study of ultrafast ordering phenomena and nucleation events is not only crucial for understanding these materials but also for the development of tools for nanoscience. With the new X-ray light sources ordering and nucleation can be investigated down to fundamental time scales of atom mobility in solids and solution, covering even short-living transient states. Research Area C is divided into three different Research Foci which focus all on time resolved investigations of ordering phenomena on the nanoscale. RFC.1 addresses the role of transient structures in molecular liquids such as water as well as the role of structural and orientational correlations for the glass transition. In RFC.2 we study nucleation and growth processes of nanoparticles and correlate their shape and phase transformations with external triggers. The subject of RFC.3 is the study of ultrafast spin ordering processes in nanostructures under the influence of dipolar and exchange interactions.

Timetable and Program

Monday, 01.12.2014

12:00	**Welcome***
12:30	**Lunch**
14:00	**Prof. Dr. P. Lucht*** *Gender Studies*
15:30	**Coffee Break**
16:00	**Ph.D. Talks:** **Session 1*** **Session 2****
17:30	**Discussion Forum I***
19:30	**Dinner**

Tuesday, 02.12.2014

08:00	**Breakfast**
09:00	**Area A:** **Prof. Dr. C. Bressler** (Basic)* **Dr. G. Steinmeyer** (Advanced)**
10:00	**Coffee Break**
10:15	**Area B:** **Prof. Dr. H. Niemann** (Basic)*
11:30	**Area C:** **Dr. R. Hertel** (Basic)* **Prof. Dr. M. Kläui** (Advanced)**
12:30	**Lunch**
14:00	**Area A:** **Prof. Dr. C. Bressler** (Basic)* **Dr. G. Steinmeyer** (Advanced)**
15:00	**Group Photo** **Free Afternoon**
19:30	**Dinner**

Wednesday, 03.12.2014

08:00	**Breakfast**
09:00	**Area A:** **Prof. Dr. C. Bressler** (Basic)* **Dr. G. Steinmeyer** (Advanced)**
10:00	**Coffee Break**
10:15	**Area B:** **Prof. Dr. H. Niemann** (Basic)*
11:30	**Area C:** **Dr. R. Hertel** (Basic)* **Prof. Dr. M. Kläui** (Advanced)**
12:30	**Lunch**
14:00	**Area A:** **Prof. Dr. C. Bressler** (Basic)* **Dr. G. Steinmeyer** (Advanced)**
15:30	**Coffee Break**
16:00	**Prof. Dr. R. Kollek*** *Societal consequences and ethical implications of new technical developments*
17:30	**Ph.D. Talks:** **Session 3*** **Session 4****
19:30	**Dinner**

Timetable and Program

Thursday, 04.12.2014

08:00	**Breakfast**
09:00	**Ph.D. Talks:** **Session 5*** **Session 6****
10:00	**Coffee Break**
10:15	**Area B:** **Prof. Dr. H. Niemann** (Basic)*
11:30	**Area C:** **Dr. R. Hertel** (Basic)* **Prof. Dr. M. Kläui** (Advanced)**
12:30	**Lunch**
14:00	**Ph.D. Talks:** **Session 7*** **Session 8****
15:30	**Coffee Break**
16:00	**Discussion Forum II***
19:30	**Dinner**

Friday, 05.12.2014

08:00	**Breakfast**
09:00	**Ph.D. Talks:** **Session 9*** **Session 10****
10:00	**Coffee Break**
10:15	**Area B:** **Prof. Dr. H. Niemann** (Basic)*
11:30	**Area C:** **Dr. R. Hertel** (Basic)* **Prof. Dr. M. Kläui** (Advanced)**
12:30	**Lunch**

Rooms:
* Schleswig
** Fehmarn

Location, Contact and Directions

Location

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Directions

By Car: Take A1 in direction of Fehmann, exit at departure Oldenburg-Mitte (Nr. 10)

By Train: take a train to Oldenburg in Holstein station, you reach the hotel by bus or taxi
(For the invited speakers a taxi service is organized)

List of Invited Speakers

Area A:

Prof. Dr. Christian Bressler (European XFEL GmbH, Hamburg)
Light-Matter Interaction

Dr. Günter Steinmeyer (Max-Born-Institut, Berlin)
Non-Linear Optics

Area B:

Prof. Dr. Hartmut Niemann (Department of Chemistry, University of Bielefeld)
Proteins - Fundamentals of the Molecular Machines in Biology

Area C:

Dr. Riccardo Hertel (Département Magnétisme des Objets NanoStructurés, IPCMS Strasbourg)
Magnetism on the atomic scale

Prof. Dr. Matthias Kläui (Institute of Physics, University of Mainz)
Static and dynamic properties of ferromagnetic nanostructures and possible applications in devices

Societal Science:

Prof. Dr. Petra Lucht
(Zentrum für Interdisziplinäre Frauen- und Geschlechterforschung, TU Berlin)
Gender Studies

Prof. Dr. Regine Kollek (FSP BIOGUM / FG Medizin, University of Hamburg)
Societal consequences and ethical implications of new technical developments

Speakers' Abstracts

Dr. Günter Steinmeyer (Max-Born-Institut, Berlin)
Non-Linear Optics

This lecture addresses nonlinear conversion of intense laser radiation in optical media. One of the most prominent nonlinear optical effects is the generation of the second harmonic at half of the wavelength of the driver radiation. This mechanism will be analyzed for the specific case of driver pulses with femtosecond temporal signature. Moreover, the lecture addresses parametric processes as well as those that follow the third power of the input power. In particular, self-refractive processes are of interest for femtosecond applications, with a spectrally overlapping input and output. The lecture will close with a discussion of current topics, like the higher-order Kerr effect and finite relaxation time constants of nonlinear optical processes.

Dr. Riccardo Hertel (Département Magnétisme des Objets NanoStructurés, IPCMS Strasbourg)
Magnetism on the atomic scale

This introductory course will provide an overview of the basic principles and properties of ferromagnetic nanostructures. The topic of the lecture series is centered around general theoretical aspects to describe the magnetization on the nanoscale, but it will also include a few experimental and computational results to illustrate particularly important features of magnetic nanostructures, domain structure formation, and dynamic magnetization processes on the nanoscale.

Lecture I: Magnetostatics and domain structures
Starting from elementary magnetostatic principles, the first lecture will focus mainly on magnetostatic fields and their representation in the case of a continuous distribution of magnetic moments. The concept of magnetostatic charges and demagnetizing factors is introduced to explain how the shape of a magnetic nanoparticle can influence its magnetic properties. The lecture will conclude with a discussion of Brown's pole avoidance principle and a simple model to anticipate the magnetic structure in soft-magnetic thin-film elements.

Lecture II: Domain walls and vortices
The second lecture will conclude the discussion on the static properties of magnetic nanostructures. This will require a basic understanding of the effect of ferromagnetic exchange and magneto-crystalline anisotropy, in addition to the magnetostatics treated in the first lecture. It will be shown how a balance of these energy terms leads to fundamental micromagnetic structures like domain walls and magnetic vortices. Certain simplifying assumptions allow for the analytic calculation of the profile of one-dimensional domain walls. A brief discussion of two-dimensional domain walls will show that the structure of real domain walls can be much more complex.

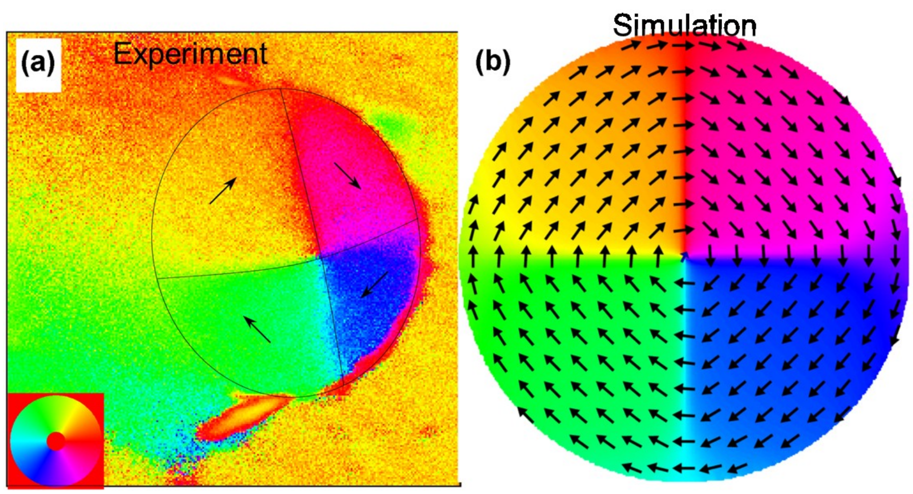
Lecture III: The Landau-Lifshitz-Gilbert Equation
The third lecture will provide an introduction into dynamic effects of the magnetization. The Landau-Lifshitz-Gilbert Equation will play a central role as the fundamental equation of motion of the magnetization. The frequently used macrospin approximation will be presented as a helpful model, which is however often too simple to capture essential features of the magnetization dynamics. Understanding the magnetization dynamics in nanostructures usually requires time-resolved high-resolution magnetic imaging and micromagnetic simulations, which will be discussed briefly.

Lecture IV: Dynamics of domain walls and vortices
The final lecture in this series will be dedicated to the dynamics of magnetic vortices and domain walls. These entities display characteristic dynamic properties that have become of great interest in the last few years, following the idea that these well-defined nanosized magnetic inhomogeneities could be promising candidates for units of information in future non-volatile devices. In this context the Walker breakdown will be discussed as a natural "speed limit" for the propagation of domain walls. A part of the lecture will address the rich variety of dynamic features that magnetic vortices can display in thin-film elements. If time permits, I will also present recent results of multiscale atomic-continuum simulations on the dynamics of Bloch points in the conclusion.

Prof. Dr. Matthias Kläui(Institute of Physics, University of Mainz)
Dr. B. Krüger(Institute of Physics, University of Mainz)
Static and dynamic properties of ferromagnetic nanostructures and possible applications in devices

In this tutorial we will introduce the physics of magnetic nanostructures and spin dynamics as well as spin currents.
We will start with an introduction of the micromagnetic model which has proven to be valuable for the description of the dynamics of magnetic systems of experimental dimensions and is valid for magnetic systems where the magnetization varies slowly in space. In the micromagnetic model the discrete magnetic moments are describe by a continuous vector field called magnetization. The different energy terms like Zeeman, exchange, demagnetization, anisotropy, and Dzyaloshinskii-Moriya interaction and their effect on the magnetization pattern will be discussed. The dynamics of the magnetization is expressed by the so called Landau–Lifshitz–Gilbert equation [1] which will be derived. It will be discussed how this equation needs to be extended to include the interaction of the magnetization with an electric current passing through the sample. We will briefly discuss how the Landau–Lifshitz–Gilbert equation can be integrated numerically to simulate the dynamics of the magnetization.

Then, we will turn to some special magnetization pattern where the solution of the Landau–Lifshitz–Gilbert equation can be approximated analytically [2] and discuss possible applications [3] of these structures. Such systems include magnetic domain walls in narrow nanowires as well as vortices and Skyrmions in thin-film elements.
This theory is applicable to cover a broad range of important applications from hard disk drives to sensors. We will discuss various experimental investigations of these nanoscale physics determining the magnetostatic spin structures and magnetodynamics of the switching [4].
Beyond using magnetic fields to manipulate magnetization, one can also use alternative approaches that exhibit better scaling. For example, when combining transport with magnetic materials on the nanoscale, a range of exciting and novel phenomena emerge. The effect of the spin polarized currents on the magnetization leads to a "spin transfer torque" effect and resulting in current-induced domain wall motion, which has become the focus of intense research in the last few years due to a strong interest in the fundamental interaction between spin – polarized currents and the magnetization in ferromagnets [5].
In current-induced domain wall motion (CIDM), due to a spin torque effect, electrons transfer angular momentum and thereby push a domain wall [5].



Comparison of an experimentally determined spin structure with a micromagnetic simulation.

[1] L. Landau and E. Lifshitz, On the Theory of the Dispersion of Magnetic Permeability in Ferromagnetic Bodies. Phys. Zeitsch. Sow. 8, 153 (1935).
[2] A. A. Thiele, Steady-State Motion of Magnetic Domains. Phys. Rev. Lett. 30, 230 (1973).
[3] S. S. P. Parkin, M. Hayashi, and L. Thomas, Magnetic Domain-Wall Racetrack Memory. Science 320, 190 (2008).
[4] M. Kläui and C. A. F. Vaz, Magnetization Configurations and Reversal in Small Magnetic Elements, Handbook of Magnetism and Advanced Magnetic Materials. Edited by Helmut Kronmüller and Stuart Parkin. Volume 2: Micromagnetism. 2007 JohnWiley & Sons, Ltd. ISBN: 978-0-470-02217-7.
[5] O. Boulle, G. Malinowski and M. Kläui, Current-induced domain wall motion in nanoscale ferromagnetic elements, Materials Science and Engineering Reports 72, 159 (2011)

Speakers' Abstracts

Prof. Dr. Petra Lucht
(Zentrum für Interdisziplinäre Frauen- und Geschlechterforschung, TU Berlin)
Gender Studies

During the last decade research institutions have begun to call for considering gender and diversity aspects in research and development of STEM fields. So far, this has been realized in multiple ways: Gender and diversity measurements and projects include e.g. the training of soft skills of scientists and engineers, improving work-life-balances or implementing organizational changes in research institutions. However, questions on how gender and diversity aspects might become integrated into the contents, the products and the applications of research and development in STEM fields mostly remain without answers.

In 2012, the Technical University Berlin started a new and highly innovative study program for students and PhD candidates in STEM fields. This study program, called Gender Pro MINT, is being offered to students in all STEM fields at the Technical University Berlin. Participating students and PhD candidates in this study program acquire gender and diversity competencies that are closely related to the contents, products and applications of research and development in STEM fields. In this study program, I am advising students for carrying out study projects and qualifying theses in project modules. In these project modules students work on reflective and inquiry-based study projects on gender and diversity in their own field of study in STEM. Students learn how to integrate approaches of gender and diversity studies into these study projects as well as into research and development projects. In most cases, these study projects and qualifying theses have been assigned to them in STEM fields (Class projects as well as Bachelor, Master or Ph.D. theses).

My talk will address the threefold approach of research-based learning and teaching on gender and diversity in STEM that I have suggested and worked with in the above mentioned project modules of the study program: Firstly, I will highlight systematic perspectives in the field of gender and diversity studies in STEM. Secondly, I will outline the research-based approach of gender and diversity training that has been developed for the project modules of the study program. A couple of examples of the students' study projects and qualifying theses in the fields of medical engineering, physics and computer science will be given. These examples show how students addressed the inclusion of gender and diversity aspects into their field of study and research in STEM. Thirdly, my presentation includes a short exercise with the audience in order to give an impression of the research-based learning approach that guides the work in the study program Gender Pro MINT at the Technical University Berlin.

For the practical exercise with the audience I would like to ask that each participant in the winter school will bring a short summary of a research project s/he is working on to the presentation.

For further information about the study program Gender Pro MINT at the Technical University Berlin see (in German): http://www.genderpromint-zifg.tu-berlin.de/

Speakers' Abstracts

Prof. Dr. Regine Kollek (FSP BIOGUM / FG Medizin, University of Hamburg)
Societal consequences and ethical implications of new technical developments

Once new scientific and/or technological developments are established in practice they will inevitable have consequences – not only the expected and desired ones, but also some which are unexpected and undesirable. This lecture starts with (and reflects on) the question why we should bother about societal and ethical implications of new technological developments. It then introduces some assumptions about the relation between science and society and the (special) responsibility of scientists. The second half of the lecture will be dedicated to technology assessment (TA). Its premises, methods and results, as well as its potentialities and limitations will be introduced. Finally, the future prospects of integrating TA in science training and research will be discussed.

Prof. Dr. Hartmut Niemann (Department of Chemistry, University of Bielefeld)
Proteins - Fundamentals of the Molecular Machines in Biology

Compared with other classes of biological (macro)molecules like DNA or sugars, the variety of functions that proteins fulfil in cells and organisms is bewilderingly complex. I will discuss why proteins are genuinely suited to perform so many different tasks. To keep it simple, the lecture will focus on a few fundamental types of molecular functions that are at the heart of this diversity.

The function of proteins is determined by their structure and by the conformational changes that they can perform. Understanding the correlation between protein structure and protein function is the primary goal of most molecular research on proteins. Therefore, I will present basic concepts of protein structure and protein folding and discuss non-covalent interactions that govern both protein folding and the interaction of proteins with binding partners.

Three experimental methods to determine the 3-dimensional structure of proteins will briefly be described, namely electron microscopy (EM), X-ray crystallography and nuclear magnetic resonance (NMR) spectroscopy. If time permits, I will also briefly touch strategies to study protein localization and function in cells and to purify proteins for in vitro studies.

Examples of various molecular machines like a turbine, a shredder and a protein-making machine will serve to illustrate the talk.

Ph.D. Talks

Area A:

Alexander Britz: (Session 5)
X-ray Probing of Electronic and Structural Correlations in Photoexcited Molecules at Synchrotrons and XFELs

Robert Büchner: (Session 1)
Chiral superfluid order of bosons in an optical lattice

Sergio Carbajo: (Session 1)
Advances towards compact relativistic electron and attosecond bright x-ray sources

Lorenzo Cardarelli: (Session 3)
Development of ML-MCTDHB(F) method

Neele Grenda: (Session 2)
Local probes for light-driven intra-molecular charge transfer

Markus Jakob: (Session 2)
Shaping of ultrashort laser pulses for controlled excitation of molecules

Jens Sebastian Kienitz: (Session 3)
Mixed-field orientation of molecules with laser pulses and very strong static electric fields

Pankaj Kumar Mishra: (Session 4)
Ultrafast Energy Transfer from Solvent to Solute induced by Sub-picosecond Highly Intense THz Pulses

Markus Pfau: (Session 4)
High-flux high-order harmonic source for time resolved molecular spectroscopy

Martin Ranke: (Session 6)
High-field terahertz generation

Joscha Reichert: (Session 7)
Dissipative Quantum Systems and Driven Baths

Bernhard Ruff: (Session 7)
Femto-second light pulses interacting with ultra-cold atoms

Johannes Schurer: (Session 8)
Many-Body Simulations of Ultracold 1D Atom-Ion Quantum Systems

Kemal Shafak: (Session 8)
Advances in Optical Timing Distribution and Synchronization Systems for X-Ray FELs

Ph.D. Talks

Vijay Pal Singh: (Session 9)
Probing superfluidity of BECs via stirring

Yudong Yang: (Session 10)
Methods of measuring attosecond pulses

Area B:

Salah Awel: (Session 1)
Optical guiding of single particles for diffractive imaging with x-ray free electron lasers

Stephanie Besztejan: (Session 2)
Metal Ions for Imaging of Dynamic Internalization Events

Zeinab Eskandarian: (Session 3)
Structural studies of Plasma-membrane Calcium ATPase

Maria Katsiaflaka: (Session 4)
Development of 2D science: the material challenge

Franziska Krawack: (Session 5)
Investigation and visualization of the translocation pore of Yersinia enterocolitica

Masoud Mehrjoo: (Session 6)
X-ray beam characterisation for Single Particle Imaging experiments at Free Electron Lasers

Julius Nitsche: (Session 7)
Structural studies of plasma-membrane Ca2+ -ATPases - an introdution

Robin Schubert: (Session 8)
Preparation of protein nano crystals and scoring by dynamic light scattering, on the basis of their radius distribution pattern

Thomas Seine: (Session 9)
Utilizing Peroxisomes as in vivo Crystal Factories

Sabrina Zinn: (Session 10)
Structure determination of trans-cinnamaldehyde using broadband-microwave spectroscopy

Ph.D. Talks

Area C:

Kai Bagschik: (Session 1)
Resonant X-ray scattering study of domain sizes in wedged multilayer samples

Eugen Klein: (Session 2)
Synthesis and structural investigation of PbS nanosheets

Jakob B. Mietner: (Session 3)
Water in Nanopores

Mona Rafipoor: (Session 4)
Highly Fluorescent non-blinking QD's and QR's

Tobias Redder: (Session 5)
In-situ experiments in a Free-Liquid Jet

Robert Seher: (Session 6)
From Clusters to Nanocrystals – Understanding early Crystallization through the use of Continous-Flow Setups

Dina Sheyfer: (Session 7)
Orientational order in glass forming fluids studied by X-ray Cross Correlation Analysis

Christian Swoboda: (Session 8)
Spin-wave excitations in deterministic fractals

Carsten Thönnißen: (Session 9)
Fabrication and measurement of single ferromagnetic nanostructures

Bright & Visionary

Organization Committee:

Dipl. Phys. Kai Bagschik

Dipl. Phys. Johannes Schurer

Graduate School:

Spokesperson: Prof. Dr. Peter Schmelcher

Coordinator: Dr. Antonio Negretti